

EXACT S MATRICES FOR INTEGRABLE QUANTUM SPIN CHAINS

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Coral Gables, FL 33124, USA**ABSTRACT**

We begin with a review of the antiferromagnetic spin $1/2$ Heisenberg chain. In particular, we show that the model has particle-like excitations with spin $1/2$, and we compute the exact bulk S matrix. We then review our recent work which generalizes these results. We first consider an integrable alternating spin $1/2$ - spin 1 chain. In addition to having excitations with spin $1/2$, this model also has excitations with spin 0 . We compute the bulk S matrix, which has some unusual features. We then consider the open antiferromagnetic spin $1/2$ Heisenberg chain with boundary magnetic fields. We give a direct calculation of the boundary S matrix. (Talk presented at the conference on Statistical Mechanics and Quantum Field Theory at USC, 16 – 21 May 1994)

1. Introduction

The investigation of integrable quantum spin chains was initiated by Bethe¹ with the classic paper on the closed * spin $1/2$ Heisenberg chain. Other examples of integrable quantum spin chains include the open spin $1/2$ chain^{2–4}, the spin 1 chain^{5,6}, the spin $1/2$ chain with a spin 1 impurity⁷, and the alternating spin $1/2$ - spin 1 chain⁸.

There are several motivations for studying integrable quantum spin chains. First, these are many-body quantum mechanical models for which exact results can be computed. Also, these models typically have^{9,10} a regime with a nontrivial

* One-dimensional quantum spin chains, like strings, come in two topologies: closed (periodic boundary conditions) and open.

antiferromagnetic vacuum and novel excitations (“spinons”). In the continuum limit, these excitations are described by 1 + 1-dimensional integrable relativistic quantum field theory. (See, e.g., Refs. 11-14.) Last but not least, such models have applications in statistical mechanics and condensed matter physics¹⁵ and perhaps also in string theory¹⁶.

In this talk we review our recent work on both bulk and boundary S matrices for the excitations of integrable quantum spin chains. Such S matrices provide valuable information about long-distance physics and boundary phenomena of the models. (See, e.g., Refs. 17, 18 and references therein.)

The outline of this talk is as follows. We begin with a brief review of the closed spin 1/2 Heisenberg chain in the antiferromagnetic regime, with emphasis on the physical properties which emerge from the Bethe Ansatz solution. In particular, following Faddeev and Takhtajan⁹, we outline the argument that the model has particle-like excitations with spin 1/2. These excitations interact, and we explain how the exact S matrix can be computed.

In the remainder of the talk, we generalize these results in two different directions. In Section 3 we consider the alternating spin 1/2 - spin 1 chain in the antiferromagnetic regime. Following Ref. 19, we show that in addition to having excitations with spin 1/2 (as in the Heisenberg chain), this model also has excitations with spin 0. We compute the S matrix, which has some unusual features. In Section 4, we consider the open antiferromagnetic spin 1/2 Heisenberg chain with boundary magnetic fields. Following Ref. 20, we give a direct calculation of the boundary S matrix. This is the first first-principles calculation of a boundary S matrix corresponding to an interacting relativistic field theory. Our result agrees with the boundary S matrix for the boundary sine-Gordon model with $\beta^2 \rightarrow 8\pi$ and with “fixed” boundary conditions^{18,21}.

2. Closed Spin 1/2 Chain

The Hamiltonian of the closed antiferromagnetic isotropic spin 1/2 Heisenberg chain is given by

$$\mathcal{H} = \frac{1}{4} \sum_{n=1}^N (\vec{\sigma}_n \cdot \vec{\sigma}_{n+1} - 1) , \quad \vec{\sigma}_{N+1} = \vec{\sigma}_1 , \quad (2.1)$$

where $\vec{\sigma}$ are the usual Pauli spin matrices. We assume that the number of spins, N , is even. The Hamiltonian commutes with the “momentum” operator P (defined

such that e^{iP} is the one-site shift operator), as well as with the $su(2)$ generators $\vec{S} = \frac{1}{2} \sum_{n=1}^N \vec{\sigma}_n$. The so-called Bethe Ansatz states are the simultaneous eigenstates of \mathcal{H} , P , S^2 and S^z which are highest weights of $su(2)$ (i.e., with corresponding eigenvalues $S = S^z \geq 0$). These states have been determined by both the coordinate¹ and algebraic²² Bethe Ansatz methods.* In the latter approach, one constructs certain creation and destruction operators, $B(\lambda)$ and $C(\lambda)$, respectively; and the Bethe Ansatz states are given by

$$B(\lambda_1) B(\lambda_2) \cdots B(\lambda_M) \omega^+, \quad (2.2)$$

where ω^+ is the ferromagnetic vacuum state with all spins up,

$$C(\lambda) \omega^+ = 0, \quad (2.3)$$

and $\{\lambda_\alpha\}$ satisfy the Bethe Ansatz (BA) equations

$$\left(\frac{\lambda_\alpha + \frac{i}{2}}{\lambda_\alpha - \frac{i}{2}} \right)^N = \prod_{\substack{\beta=1 \\ \beta \neq \alpha}}^M \left(\frac{\lambda_\alpha - \lambda_\beta + i}{\lambda_\alpha - \lambda_\beta - i} \right), \quad \alpha = 1, \dots, M, \quad M \leq \frac{N}{2}. \quad (2.4)$$

The corresponding eigenvalues are given by

$$\begin{aligned} E &= -\frac{1}{2} \sum_{\alpha=1}^M \frac{1}{\lambda_\alpha^2 + \frac{1}{4}}, \\ P &= \frac{1}{i} \sum_{\alpha=1}^M \log \left(\frac{\lambda_\alpha + \frac{i}{2}}{\lambda_\alpha - \frac{i}{2}} \right), \\ S = S^z &= \frac{N}{2} - M. \end{aligned} \quad (2.5)$$

For the ferromagnetic spin chain with Hamiltonian $-\mathcal{H}$, the ground state has all spins aligned, and evidently corresponds to $M = 0$. For the antiferromagnetic spin chain with Hamiltonian $+\mathcal{H}$ (2.1), the identification of the ground state and the lowest-lying excited states is as follows:

* The remaining states are obtained by acting on the Bethe Ansatz states with the spin lowering operator S^- .

2.1 Ground state

For the ground state, one can argue that $M = \frac{N}{2}$ and that the roots $\{\lambda_1, \dots, \lambda_M\}$ are all distinct and real. This solution of the BA equations corresponds to a filled Fermi sea (i.e., no holes). See Fig. 1.

For $N \rightarrow \infty$, the set of λ 's becomes dense on the real line, and is described by the density $\sigma_{vac}(\lambda)$ which is given by*

$$\sigma_{vac}(\lambda) = \frac{1}{2 \cosh \pi \lambda} + O\left(\frac{1}{N^2}\right). \quad (2.6)$$

(This result is obtained by solving the linear integral equation for the root density which follows from the BA equations.) Making in Eq. (2.5) the following replacement of sums by integrals

$$\frac{1}{N} \sum_{\alpha=1}^M () \rightarrow \int_{-\infty}^{\infty} () \sigma_{vac}(\lambda) d\lambda, \quad (2.7)$$

one concludes that the ground state has the following quantum numbers:

$$E = E_0 = -N \log 2, \quad P = P_0 = N\pi/2, \quad S = 0. \quad (2.8)$$

In particular, the ground state is a spin singlet, as one would expect for an antiferromagnet.

2.2 Excitations

The excited states above the ground state consist of an even number of particle-like excitations, which are now known as “spinons”. (Faddeev-Takhtajan called them “kinks”.) Therefore, the lowest-lying excited states have two spinons. One can argue that there are four such states: the triplet ($S = 1$) states, and the singlet ($S = 0$) state. (The total number of states with ν spinons is equal to 2^ν .) The fact that the excited states with two spinons have $S = 1$ and $S = 0$ implies the important result that a spinon has spin $1/2$.

The triplet state with $S = S^z = 1$ is described by only real roots $\{\lambda_1, \dots, \lambda_M\}$ (as is the ground state), but with $M = \frac{N}{2} - 1$. This solution of the BA equations corresponds to a Fermi sea with two holes. The hole rapidities are labeled $\tilde{\lambda}_1, \tilde{\lambda}_2$. See Fig. 2.

* The Fermi points are at $\pm\infty$. Had we introduced a bulk magnetic field, the Fermi points would be at $\lambda = \pm\Lambda$, with Λ finite.

The singlet state corresponds to a Fermi sea with two holes (with rapidities $\tilde{\lambda}_1$ and $\tilde{\lambda}_2$) as well as a “2 - string”, which is a set of conjugate roots $\lambda_0 \pm \frac{i}{2}$, with λ_0 (the “center” of the 2 - string) real. For the singlet state, the BA equations further constrain the center to be given by

$$\lambda_0 = \frac{1}{2}(\tilde{\lambda}_1 + \tilde{\lambda}_2). \quad (2.9)$$

All of these features of the singlet-state solution can be seen in Fig. 3.

For both the triplet and singlet states, one can show that the density $\sigma(\lambda)$ of real roots and holes is given by an expression of the form

$$\sigma(\lambda) = \frac{1}{2 \cosh \pi \lambda} + \frac{1}{N} r(\lambda) + O\left(\frac{1}{N^2}\right), \quad (2.10)$$

where $r(\lambda)$ is a correction of order 1 to the ground state density (2.6). Heuristically, this correction corresponds to a “polarization” of the Fermi sea due to the holes and the 2-string. Explicitly,

$$\begin{aligned} r_{\text{triplet}}(\lambda) &= \sum_{\alpha=1}^2 J(\lambda - \tilde{\lambda}_\alpha), \\ r_{\text{singlet}}(\lambda) &= r_{\text{triplet}}(\lambda) - a_1(\lambda - \lambda_0), \end{aligned} \quad (2.11)$$

where

$$J(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, e^{-i\omega\lambda} \frac{e^{-|\omega|}}{1 + e^{-|\omega|}}, \quad a_1(\lambda) = \frac{i}{2\pi} \frac{d}{d\lambda} \log \left(\frac{\lambda + \frac{i}{2}}{\lambda - \frac{i}{2}} \right). \quad (2.12)$$

It follows from Eq. (2.5) that for both the triplet and singlet states, the energy and momentum are given by

$$\begin{aligned} E &= E_0 + \varepsilon(\tilde{\lambda}_1) + \varepsilon(\tilde{\lambda}_2), \\ P &= P_0 + p(\tilde{\lambda}_1) + p(\tilde{\lambda}_2), \end{aligned} \quad (2.13)$$

where E_0 and P_0 are the energy and momentum of the ground state, and

$$\varepsilon(\lambda) = \frac{\pi}{2 \cosh \pi \lambda}, \quad (2.14)$$

$$p(\lambda) = \tan^{-1} \sinh \pi \lambda - \frac{\pi}{2}. \quad (2.15)$$

From the additivity property displayed by Eq. (2.13), we see that the spinons indeed are particle-like excitations, with energy $\varepsilon(\lambda)$ and momentum $p(\lambda)$. The energy-momentum dispersion relation is

$$\varepsilon = -\frac{\pi}{2} \sin p. \quad (2.16)$$

Note that the spinons are gapless ($\varepsilon(\lambda) \rightarrow 0$ for $\lambda \rightarrow \pm\infty$).

2.3 S matrix

The S matrix for the scattering of spinons can be calculated exactly. Here we follow the Korepin-Andrei-Destri^{23,24} method. An important observation is that for a state of two spinons with rapidities $\tilde{\lambda}_1$ and $\tilde{\lambda}_2$, the momentum $p(\tilde{\lambda}_1)$ satisfies the quantization condition

$$e^{ip(\tilde{\lambda}_1)N} \check{R}(\tilde{\lambda}_1 - \tilde{\lambda}_2) = 1, \quad (2.17)$$

where \check{R} is the 2-particle S matrix (acting in the tensor product space $C^2 \otimes C^2$), and N is the number of spins in the chain. Let $e^{i\phi}$ be an eigenvalue of \check{R} . Then $p(\tilde{\lambda}_1)$ is related to the phase shift ϕ by

$$p(\tilde{\lambda}_1) + \frac{1}{N}\phi = \frac{2\pi}{N}m, \quad (2.18)$$

where m is an integer.

On the other hand, one can show that

$$p(\tilde{\lambda}_1) + \frac{2\pi}{N} \int_{-\infty}^{\tilde{\lambda}_1} r(\lambda) d\lambda + const = \frac{2\pi}{N} \tilde{J}_1, \quad (2.19)$$

where $r(\lambda)$ is the function appearing in Eq. (2.10), and \tilde{J}_1 is an integer or half-odd integer. Comparing Eqs. (2.18) and (2.19), we conclude that the phase shift ϕ is given by

$$\phi = 2\pi \int_{-\infty}^{\tilde{\lambda}_1} r(\lambda) d\lambda + const. \quad (2.20)$$

Using the explicit expressions for $r(\lambda)$ for the triplet and singlet states, we obtain (up to a rapidity-independent phase factor)

$$\begin{aligned} S_{triplet}(\lambda) &= e^{i\phi_{triplet}} = \frac{\Gamma(1 + \frac{i\lambda}{2})\Gamma(\frac{1}{2} - \frac{i\lambda}{2})}{\Gamma(1 - \frac{i\lambda}{2})\Gamma(\frac{1}{2} + \frac{i\lambda}{2})}, \\ S_{singlet}(\lambda) &= e^{i\phi_{singlet}} = -\frac{\lambda + i}{\lambda - i} S_{triplet}(\lambda), \end{aligned} \quad (2.21)$$

where $\lambda = \tilde{\lambda}_1 - \tilde{\lambda}_2$.

2.4 Further remarks

It is useful to formulate the above result as a 4×4 matrix. Since \check{R} commutes with $su(2)$, it is a linear combination of the identity matrix 1 and the permutation matrix \mathcal{P} . Moreover, \check{R} has the eigenvalues (2.21). It follows that

$$R(\lambda) \equiv \mathcal{P}\check{R}(\lambda) = \frac{\Gamma(1 + \frac{i\lambda}{2})\Gamma(\frac{1}{2} - \frac{i\lambda}{2})}{\Gamma(1 - \frac{i\lambda}{2})\Gamma(\frac{1}{2} + \frac{i\lambda}{2})} \frac{(\lambda 1 - i\mathcal{P})}{(\lambda - i)}. \quad (2.22)$$

The matrix R satisfies unitarity and crossing, as well as the Yang-Baxter equation

$$R_{12}(\lambda - \lambda') R_{13}(\lambda) R_{23}(\lambda') = R_{23}(\lambda') R_{13}(\lambda) R_{12}(\lambda - \lambda'), \quad (2.23)$$

where R_{12} , R_{13} , and R_{23} are matrices acting in the tensor product space $C^2 \otimes C^2 \otimes C^2$, with $R_{12} = R \otimes 1$, $R_{23} = 1 \otimes R$, etc. (See, e.g., Refs. 17, 25 and references therein.)

We have described here only the calculation of the 2-particle S matrix. In principle one can compute in similar fashion the multiparticle S matrix, and verify that the multiparticle S matrix is factorizable into a product of 2-particle S matrices.

Finally, we briefly discuss the continuum limit of this model. The continuum quantum field theory is²⁶ the $su(2)$ WZW model²⁷ of level $k = 1$. This is an $su(2)$ -invariant CFT²⁸ with central charge $c = 1$. Indeed, the massless S matrix¹³ of the latter model coincides with Eq. (2.21).

The S matrix (2.21) can also be obtained by starting with an anisotropic spin chain with anisotropy parameter η and lattice spacing a , and then taking the continuum limit $a \rightarrow 0$ and the isotropic limit $\eta \rightarrow 0$ while keeping a mass parameter $m^2 \propto a^{-2} \exp(-\pi^2/\eta)$ fixed. (See Ref. 11.) Thus, this S matrix also describes a massive $su(2)$ -invariant integrable quantum field theory (namely¹⁷, the $su(2)$ -invariant Thirring model, or the sine-Gordon model in the limit $\beta^2 \rightarrow 8\pi$), which in the ultraviolet limit $m \rightarrow 0$ reduces to the WZW model.

3. Closed Alternating Spin 1/2 - Spin 1 Chain

We now consider a system with a strictly alternating arrangement of $2N$ spins, with spins $1/2$ at even sites and spins 1 at odd sites. That is, there are N spins $\frac{1}{2}\vec{\sigma}_2, \frac{1}{2}\vec{\sigma}_4, \dots, \frac{1}{2}\vec{\sigma}_{2N}$ of spin $1/2$ and N spins $\vec{s}_1, \vec{s}_3, \dots, \vec{s}_{2N-1}$ of spin 1 . The $su(2)$ -invariant Hamiltonian \mathcal{H} is given by^{8,29}

$$\mathcal{H} = -\frac{1}{18} \sum_{n=1}^N \left\{ (2\vec{\sigma}_{2n} \cdot \vec{s}_{2n+1} + 1) (2\vec{\sigma}_{2n+2} \cdot \vec{s}_{2n+1} + 3) \right. \quad (3.1)$$

$$+ (2\vec{\sigma}_{2n} \cdot \vec{s}_{2n-1} + 1) [(1 + \vec{s}_{2n-1} \cdot \vec{s}_{2n+1}) (2\vec{\sigma}_{2n} \cdot \vec{s}_{2n+1} + 1) + 2] \Big\}.$$

Note that the Hamiltonian contains both nearest and next-to-nearest neighbor interactions. We assume periodic boundary conditions ($\vec{\sigma}_{2n} \equiv \vec{\sigma}_{2n+2N}$ and $\vec{s}_{2n+1} \equiv \vec{s}_{2n+1+2N}$) and that N is even.

It is not difficult to understand the origin of this Hamiltonian. Using R matrices* $R^{(\frac{1}{2}, \frac{1}{2})}$, $R^{(\frac{1}{2}, 1)}$, $R^{(1, \frac{1}{2})}$ and $R^{(1, 1)}$ as vertex weights, one can construct⁸ an integrable two-dimensional classical statistical mechanical vertex model as shown in Fig. 4. Note that both rows and columns alternate between spin 1/2 and spin 1, and that the lattice is invariant under rotation by $\pi/2$. The logarithmic derivative of the (two-row to two-row) transfer matrix gives the above Hamiltonian.

The Bethe Ansatz states have been determined in Ref. 8. The corresponding energy, momentum, and spin eigenvalues are given by

$$\begin{aligned} E &= - \sum_{\alpha=1}^M \left(\frac{1}{2} \frac{1}{\lambda_{\alpha}^2 + \frac{1}{4}} + \frac{1}{\lambda_{\alpha}^2 + 1} \right) + \text{independent of } \{\lambda_{\alpha}\}, \\ P &= \frac{1}{2i} \sum_{\alpha=1}^M \log \left(\frac{\lambda_{\alpha} + \frac{i}{2}}{\lambda_{\alpha} - \frac{i}{2}} \frac{\lambda_{\alpha} + i}{\lambda_{\alpha} - i} \right), \\ S &= S^z = \frac{3N}{2} - M, \end{aligned} \tag{3.2}$$

where the variables λ_{α} satisfy the BA equations

$$\left(\frac{\lambda_{\alpha} + \frac{i}{2}}{\lambda_{\alpha} - \frac{i}{2}} \frac{\lambda_{\alpha} + i}{\lambda_{\alpha} - i} \right)^N = \prod_{\substack{\beta=1 \\ \beta \neq \alpha}}^M \frac{\lambda_{\alpha} - \lambda_{\beta} + i}{\lambda_{\alpha} - \lambda_{\beta} - i}, \quad \alpha = 1, \dots, M, \quad M \leq \frac{3N}{2}. \tag{3.3}$$

The momentum operator is defined such that e^{i2P} is the two-site shift operator, and hence the factor 1/2 in Eq. (3.2).

The ground state corresponds to *two* filled Fermi seas: a sea of 1-strings (i.e., real roots of the BA equations, as in the ground state of the spin 1/2 chain) and a sea of 2-strings. See Fig. 5.

Holes in the sea of 2-strings are excitations with spin 1/2, just like the excitations of the spin 1/2 chain. However, for the alternating spin chain, there is the additional possibility of having holes in the sea of 1-strings. As shown in Ref.

* We denote by $R^{(s_1, s_2)}(\lambda)$ the $su(2)$ -invariant R matrix acting on the tensor product space $C^{2s_1+1} \otimes C^{2s_2+1}$ corresponding to spins s_1 and s_2 . See Refs. 5, 30.

19, holes in the sea of 1-strings are excitations with spin 0. To the best of our knowledge, this is the first example of a magnetic chain with spin 0 excitations.

For both the spin 1/2 and spin 0 excitations, the energy $\varepsilon(\lambda)$ is given by (2.14), and the momentum is given $p(\lambda)/2$, where $p(\lambda)$ is given by (2.15). The total number of states with ν excitations is $\sum_{m=0}^{\nu/2} 2^{2m}$, which corresponds to having an even number of each type of excitation.

The S matrix can be computed (up to rapidity-independent phase factors) as before. The triplet and singlet S matrix elements for the scattering of two spin 1/2 excitations coincide with the expressions given in Eq. (2.21). There is no scattering between two spin 0 excitations (the S matrix element is $S(\lambda) = 1$) and the S matrix element for the scattering of a spin 1/2 excitation and a spin 0 excitation is

$$S(\lambda) = i \coth \frac{\pi}{2} \left(\lambda + \frac{i}{2} \right), \quad (3.4)$$

where λ is the difference of the corresponding hole rapidities. Remarkably, the scalar-spinor scattering is nontrivial, yet the spinor-spinor scattering is the same as for the Heisenberg chain.

An interesting open problem is to determine the continuum limit of this model. We know that the continuum quantum field theory must be some $su(2)$ -invariant CFT with^{29,31} central charge $c = 2$.

We remark that for both the spin 1/2 chain and the alternating spin 1/2 - spin 1 chain, the ratio C_H/T (the specific heat at constant field divided by the temperature) has the property

$$\lim_{T \rightarrow 0} \lim_{H \rightarrow 0} \frac{C_H}{T} = \lim_{H \rightarrow 0} \lim_{T \rightarrow 0} \frac{C_H}{T}. \quad (3.5)$$

The LHS can be evaluated by the method of Filyov, *et al.*³² while the RHS can be evaluated by the method of Johnson and McCoy³³.

For integrable isotropic spin s chains with $s > 1/2$ ^{30,34,35}, the property (3.5) is not satisfied. Indeed, the LHS is proportional to $c = 3s/(s+1)$ (see Ref. 26), while the RHS is proportional to $c = 1$ (see Ref. 36). Moreover, there is a discrepancy between the results of Takhtajan³⁴ (see also Ref. 24) and Reshetikhin³⁷ for the two-body S matrix:

$$S_{\text{Takhtajan}} \neq S_{\text{Reshetikhin}}. \quad (3.6)$$

These facts strongly suggest that there are (at least) two continuous field theories in the $(T, H) = (0, 0)$ limit of the spin s isotropic chain. The limit $T = 0, H = 0^+$

corresponds to a $c = 1$ theory with Takhtajan's S matrix; and the limit $H = 0, T = 0^+$ corresponds to a $c = 3s/(s+1)$ theory with Reshetikhin's S matrix.

4. Open Spin 1/2 Chain with Boundary Magnetic Fields

We now consider the open antiferromagnetic isotropic spin 1/2 Heisenberg chain with boundary magnetic fields. The Hamiltonian is given by

$$\mathcal{H} = \frac{1}{4} \left\{ \sum_{n=1}^N \vec{\sigma}_n \cdot \vec{\sigma}_{n+1} + \frac{1}{\xi_-} \sigma_1^z + \frac{1}{\xi_+} \sigma_N^z \right\}, \quad (4.1)$$

where the (real) parameters ξ_{\pm} correspond to boundary magnetic fields. We assume that $\xi_{\pm} > 1/2$ and that N is even. Since the spin chain is open, the Hamiltonian does not commute with the shift operator. Moreover, the boundary magnetic fields break the $su(2)$ symmetry, and so the Hamiltonian commutes only with S^z .

The simultaneous eigenstates of \mathcal{H} and S^z have been determined by both the coordinate³ and algebraic⁴ Bethe Ansatz. In the latter approach, one constructs (in analogy with the closed spin chain) certain creation and destruction operators, $\mathcal{B}(\lambda)$ and $\mathcal{C}(\lambda)$, respectively; and the eigenstates are given by

$$\mathcal{B}(\lambda_1) \mathcal{B}(\lambda_2) \cdots \mathcal{B}(\lambda_M) \omega^+, \quad (4.2)$$

where ω^+ is the ferromagnetic vacuum state with all spins up,

$$\mathcal{C}(\lambda) \omega^+ = 0, \quad (4.3)$$

and $\{\lambda_{\alpha}\}$ satisfy the Bethe Ansatz (BA) equations

$$\begin{aligned} & \left(\frac{\lambda_{\alpha} + i(\xi_+ - \frac{1}{2})}{\lambda_{\alpha} - i(\xi_+ - \frac{1}{2})} \right) \left(\frac{\lambda_{\alpha} + i(\xi_- - \frac{1}{2})}{\lambda_{\alpha} - i(\xi_- - \frac{1}{2})} \right) \left(\frac{\lambda_{\alpha} + \frac{i}{2}}{\lambda_{\alpha} - \frac{i}{2}} \right)^{2N} \\ &= \prod_{\substack{\beta=1 \\ \beta \neq \alpha}}^M \left(\frac{\lambda_{\alpha} - \lambda_{\beta} + i}{\lambda_{\alpha} - \lambda_{\beta} - i} \right) \left(\frac{\lambda_{\alpha} + \lambda_{\beta} + i}{\lambda_{\alpha} + \lambda_{\beta} - i} \right), \quad \alpha = 1, \dots, M. \end{aligned} \quad (4.4)$$

The corresponding energy and spin eigenvalues are given by

$$E = -\frac{1}{2} \sum_{\alpha=1}^M \frac{1}{\lambda_{\alpha}^2 + \frac{1}{4}} + \text{independent of } \{\lambda_{\alpha}\}, \quad (4.5)$$

$$S^z = \frac{N}{2} - M. \quad (4.6)$$

We require that the BA solutions correspond to independent BA states, and therefore, we make the restriction

$$\text{Re}(\lambda_\alpha) > 0. \quad (4.7)$$

(See, e.g., Refs. 2, 3, 20, 21, 38, 39.)

As for the closed spin 1/2 chain, the ground state corresponds to a real Fermi sea, and the excitations are spinons with $S^z = \pm 1/2$ and energy $\varepsilon(\lambda)$. We assume that the 2-particle S matrix is the same as for the closed spin chain. The problem is to compute the boundary S matrix, which describes the interaction of a spinon with the end of the spin chain. However, it is instructive to first consider a similar but more elementary problem.

4.1 Boundary S matrix: free particle

As a warm-up exercise, we first compute the boundary S matrix for a free non-relativistic particle of mass m (with Hamiltonian $H = p^2/2m$) which is constrained to be on the positive half-line $x \geq 0$. Usually one demands that the wavefunction $\psi(x)$ vanish at $x = 0$. This is a sufficient, but by no means necessary, condition for the probability current $j(x) = i\psi(x)^* \overleftrightarrow{\partial}_x \psi(x)$ to vanish at $x = 0$. We consider instead the more general (mixed Dirichlet-Neumann) boundary condition

$$c\psi(x) + \frac{d}{dx}\psi(x) = 0 \quad \text{at } x = 0, \quad (4.8)$$

where c is a real parameter with dimension 1/length. This boundary condition also implies the vanishing of the probability current at $x = 0$, and is compatible with the self-adjointness of the Hamiltonian. (This boundary condition has been shown⁴⁰ to be compatible with the integrability of the nonlinear Schrödinger equation on the positive half-line.) Assuming energy eigenfunctions of the plane-wave form

$$\psi_p(x) = Ae^{ipx} + Be^{-ipx} \quad (4.9)$$

(we set $\hbar = 1$), we can use the boundary condition (4.8) to eliminate A in terms of B ; and we immediately obtain

$$\psi_p(x) = B \left[e^{-ipx} + \left(\frac{p + ic}{p - ic} \right) e^{ipx} \right]. \quad (4.10)$$

We conclude that the boundary S matrix is given by

$$K(p) = \frac{p + ic}{p - ic}. \quad (4.11)$$

We see that the boundary can give rise to a nontrivial boundary S matrix. The pole at $p = ic$ implies the existence (for $c > 0$) of a boundary bound state with energy $E = -c^2/2m$.

4.2 Boundary S matrix: open spin 1/2 chain

For the open spin 1/2 chain, the quantization condition (2.17) is replaced by²¹

$$e^{i2p(\tilde{\lambda}_1)N} R_{12}(\tilde{\lambda}_1 - \tilde{\lambda}_2) K_1(\tilde{\lambda}_1, \xi_-) R_{21}(\tilde{\lambda}_1 + \tilde{\lambda}_2) K_1(\tilde{\lambda}_1, \xi_+) = 1. \quad (4.12)$$

Here $p(\lambda)$ is defined by (2.15) (i.e, the expression for the momentum of a particle with rapidity λ for the corresponding system with periodic boundary conditions), and $K(\lambda, \xi)$ is the boundary S matrix (acting in the space C^2). We use the same notation employed in Eq. (2.23); moreover,

$$R_{21}(\lambda) \equiv \mathcal{P}_{12} R_{12}(\lambda) \mathcal{P}_{12}, \quad (4.13)$$

where \mathcal{P} is the permutation matrix; and K_1, K_2 denote matrices acting in the space $C^2 \otimes C^2$, with $K_1 = K \otimes 1, K_2 = 1 \otimes K$.

The R matrix is given in Eq. (2.22). This matrix has the following form

$$R(\lambda) = \begin{pmatrix} a(\lambda) & 0 & 0 & 0 \\ 0 & b(\lambda) & c(\lambda) & 0 \\ 0 & c(\lambda) & b(\lambda) & 0 \\ 0 & 0 & 0 & a(\lambda) \end{pmatrix}, \quad (4.14)$$

with

$$b(\lambda) = \frac{\lambda}{\lambda - i} a(\lambda), \quad c(\lambda) = -\frac{i}{\lambda - i} a(\lambda), \quad a(\lambda) = \frac{\Gamma(1 + \frac{i\lambda}{2})\Gamma(\frac{1}{2} - \frac{i\lambda}{2})}{\Gamma(1 - \frac{i\lambda}{2})\Gamma(\frac{1}{2} + \frac{i\lambda}{2})}.$$

The $U(1)$ symmetry of the Hamiltonian's boundary terms implies that the boundary S matrix is of the form

$$K(\lambda, \xi) = \begin{pmatrix} \alpha(\lambda, \xi) & 0 \\ 0 & \beta(\lambda, \xi) \end{pmatrix}. \quad (4.15)$$

Our task is to explicitly determine the matrix elements $\alpha(\lambda, \xi)$ and $\beta(\lambda, \xi)$, which are the boundary scattering amplitudes for excitations with $S^z = +1/2$ and $S^z = -1/2$, respectively. We proceed by examining the two-particle excited states, which we classify by their S^z eigenvalue. As for the closed spin 1/2 chain, there are four such states ($S^z = 1, S^z = -1$, and two states with $S^z = 0$). Since we need

to determine only two matrix elements, the system of four equations provided by the quantization condition (4.12) is overdetermined. The structure (4.14) of the R matrix suggests that there will be two simple relations corresponding to the diagonal elements of the R matrix. These relations will enable us to determine the matrix elements $\alpha(\lambda, \xi)$ and $\beta(\lambda, \xi)$. The other two relations should lead to identities.

$S^z = 1$ state

For the $S^z = 1$ state, the quantization condition (4.12) implies

$$2p(\tilde{\lambda}_1) + \frac{1}{N}\Phi^{(1)} = \frac{2\pi}{N}m, \quad (4.16)$$

with

$$e^{i\Phi^{(1)}} = a(\tilde{\lambda}_1 - \tilde{\lambda}_2) \alpha(\tilde{\lambda}_1, \xi_-) a(\tilde{\lambda}_1 + \tilde{\lambda}_2) \alpha(\tilde{\lambda}_1, \xi_+). \quad (4.17)$$

As for the closed spin chain, the $S^z = 1$ state is the Bethe Ansatz state consisting of two holes in the (real) Fermi sea. Using the BA equations, we can compute²⁰ the function $r(\lambda)$, which is the sum of $1/N$ contributions to the density $\sigma(\lambda)$ for this state.* For the open spin chain, the identity (2.19) is replaced by

$$2p(\tilde{\lambda}_1) + \frac{2\pi}{N} \int_0^{\tilde{\lambda}_1} r(\lambda) d\lambda + const = \frac{2\pi}{N} \tilde{J}_1. \quad (4.18)$$

It follows that

$$\Phi^{(1)} = 2\pi \int_0^{\tilde{\lambda}_1} r(\lambda) d\lambda + const. \quad (4.19)$$

Using the explicit expressions for $r(\lambda)$ and $a(\lambda)$, we obtain the following result for $\alpha(\lambda, \xi)$ (up to a rapidity-independent phase factor):

$$\alpha(\lambda, \xi) = \frac{\Gamma\left(\frac{-i\lambda}{2} + \frac{1}{4}\right)}{\Gamma\left(\frac{i\lambda}{2} + \frac{1}{4}\right)} \frac{\Gamma\left(\frac{i\lambda}{2} + 1\right)}{\Gamma\left(\frac{-i\lambda}{2} + 1\right)} \frac{\Gamma\left(\frac{-i\lambda}{2} + \frac{1}{4}(2\xi - 1)\right)}{\Gamma\left(\frac{i\lambda}{2} + \frac{1}{4}(2\xi - 1)\right)} \frac{\Gamma\left(\frac{i\lambda}{2} + \frac{1}{4}(2\xi + 1)\right)}{\Gamma\left(\frac{-i\lambda}{2} + \frac{1}{4}(2\xi + 1)\right)}. \quad (4.20)$$

$S^z = -1$ state

To determine the remaining element $\beta(\lambda, \xi)$ of the boundary S matrix, we consider the $S^z = -1$ state. The quantization condition (4.12) implies

$$2p(\tilde{\lambda}_1) + \frac{1}{N}\Phi^{(-1)} = \frac{2\pi}{N}m, \quad (4.21)$$

* In contrast to the closed-chain result (2.6), the ground-state density $\sigma_{vac}(\lambda)$ for the open spin chain has corrections of order $1/N$, and these corrections contribute to $r(\lambda)$.

with

$$e^{i\Phi^{(-1)}} = a(\tilde{\lambda}_1 - \tilde{\lambda}_2) \beta(\tilde{\lambda}_1, \xi_-) a(\tilde{\lambda}_1 + \tilde{\lambda}_2) \beta(\tilde{\lambda}_1, \xi_+). \quad (4.22)$$

The $S^z = -1$ state is most easily described within the BA approach by changing the pseudovacuum. Hence, instead of working with the states (4.2), we work now with

$$\mathcal{C}(\lambda_1) \mathcal{C}(\lambda_2) \cdots \mathcal{C}(\lambda_M) \omega^-, \quad (4.23)$$

where ω^- is the ferromagnetic vacuum state with all spins down,

$$\mathcal{B}(\lambda) \omega^- = 0. \quad (4.24)$$

Sklyanin has shown⁴ that $\{\lambda_\alpha\}$ in Eq. (4.23) satisfy the same BA equations (4.4) as before, except for the replacement of ξ_\pm by $-\xi_\pm$. The energy eigenvalues are given by the same expression (4.5), and the S^z eigenvalues are now given by

$$S^z = M - \frac{N}{2}. \quad (4.25)$$

The $S^z = -1$ state now corresponds to the Bethe Ansatz state consisting of two holes in the Fermi sea. The calculation of the function $r(\lambda)$ is exactly the same as for the $S^z = 1$ state, except that we must track the change $\xi_\pm \rightarrow -\xi_\pm$. We find that $\beta(\lambda, \xi)$ is given by

$$\beta(\lambda, \xi) = -\frac{\lambda + i(\xi - \frac{1}{2})}{\lambda - i(\xi - \frac{1}{2})} \alpha(\lambda, \xi), \quad (4.26)$$

where $\alpha(\lambda, \xi)$ is given by Eq. (4.20). This completes the derivation of the boundary S matrix.

$S^z = 0$ states

We have already succeeded to determine the boundary S matrix. Nevertheless, a good check on this result and on the general formalism is provided by analyzing the $S^z = 0$ states, of which there are two. In particular, we consider the $S^z = 0$ state consisting of two holes in the Fermi sea, and also one 2-string. For $\xi_\pm \rightarrow \infty$, this is the spin-singlet ($S = S^z = 0$) state shown in Fig. 6. *

* The other $S^z = 0$ state is the one which for $\xi_\pm \rightarrow \infty$ is one of the spin triplet ($S = 1$) states. For $\xi_\pm \neq \infty$, it is not clear how to identify this state in terms of the Bethe Ansatz solution, and we do not consider it further.

the center of the 2-string is *not* given by the simple expression (2.9). For example, for the special case $\xi_{\pm} = \infty$, the center position is

$$\lambda_0 = \sqrt{\frac{1}{4} + \frac{1}{2} [(\tilde{\lambda}_1)^2 + (\tilde{\lambda}_2)^2]}. \quad (4.27)$$

The general case $\xi_{\pm} \neq \infty$ is discussed in Ref. 20.

For the $S^z = 0$ states, the quantization condition (4.12) leads to a 2×2 matrix equation. The two eigenvalues of this matrix are pure phases. Since the matrix elements of $R(\lambda)$ and $K(\lambda, \xi_{\pm})$ are known, these eigenvalues can be computed explicitly. Let $\exp i\Phi^{(0)}$ be the eigenvalue which for $\xi_{\pm} \rightarrow \infty$ corresponds to the spin-singlet ($S = S^z = 0$) state. The quantization condition implies

$$e^{i2p(\tilde{\lambda}_1)N} e^{i\Phi^{(0)}} = 1. \quad (4.28)$$

From Eq. (4.18) and the corresponding function $r(\lambda)$, we obtain the consistency condition

$$e^{i(\Phi^{(0)} - \Phi^{(1)})} = e_1(\tilde{\lambda}_1 - \lambda_0) e_1(\tilde{\lambda}_1 + \lambda_0), \quad (4.29)$$

where

$$e_1(\lambda) = \frac{\lambda + \frac{i}{2}}{\lambda - \frac{i}{2}}, \quad (4.30)$$

$\Phi^{(1)}$ is defined in (4.17), the hole rapidities $\tilde{\lambda}_1$ and $\tilde{\lambda}_2$ are arbitrary, and λ_0 is the corresponding rapidity of the center of the 2-string.

For the case $\xi_{\pm} = \infty$, this relation is satisfied by virtue of the algebraic identity

$$e_1\left(\frac{1}{2}(\tilde{\lambda}_1 - \tilde{\lambda}_2)\right) e_1\left(\frac{1}{2}(\tilde{\lambda}_1 + \tilde{\lambda}_2)\right) = e_1(\tilde{\lambda}_1 - \lambda_0) e_1(\tilde{\lambda}_1 + \lambda_0). \quad (4.31)$$

which is true for arbitrary values of $\tilde{\lambda}_1$ and $\tilde{\lambda}_2$, where λ_0 is given by (4.27). We have explicitly verified the formula (4.29) also for the case $\xi_- = \infty$, $\xi_+ \neq \infty$, and presumably it is true in general. This equality provides a nontrivial consistency check of the bulk and boundary S matrices and of the general formalism.

4.3 Further remarks

The boundary S matrix $K(\lambda, \xi)$ given by Eqs. (4.15), (4.20), (4.26) satisfies boundary unitarity and boundary cross-unitarity¹⁸, as well as the boundary Yang-Baxter equation^{4,18,41,42}

$$R_{12}(\lambda - \lambda') K_1(\lambda, \xi) R_{21}(\lambda + \lambda') K_2(\lambda', \xi) = K_2(\lambda', \xi) R_{12}(\lambda + \lambda') K_1(\lambda, \xi) R_{21}(\lambda - \lambda'). \quad (4.32)$$

Since the bulk S matrix coincides with that of the sine-Gordon model with $\beta^2 \rightarrow 8\pi$, we expect that the boundary S matrix $K(\lambda, \xi)$ should coincide with the boundary S matrix of Ghoshal and Zamolodchikov¹⁸ for the boundary sine-Gordon model with $\beta^2 \rightarrow 8\pi$ and with “fixed” boundary conditions. (For “fixed” boundary conditions, the field theory and hence the boundary S matrix are $U(1)$ invariant.) We have verified that the two boundary S matrices indeed coincide, up to a rapidity-independent scalar factor, and with some redefinitions of variables. The bootstrap result of Ghoshal and Zamolodchikov for the boundary sine-Gordon model with “fixed” boundary conditions has been verified using the physical Bethe Ansatz approach by Fendley and Saleur²¹. Very recently, the boundary S matrix for the anisotropic spin 1/2 chain has been calculated by Jimbo, *et al.*⁴³ using the vertex operator approach. In the isotropic limit, their result coincides with ours.

We have seen that the analysis of the $S^z = 0$ states for the open spin chain differs significantly from that of the closed spin chain. Indeed, for the open chain, the position of the center of the 2-string is a complicated function of the hole rapidities $\tilde{\lambda}_1$ and $\tilde{\lambda}_2$ (as well as the boundary parameters ξ_{\pm}); while for the closed chain, the center of the string is located midway between the two holes. Naively, one might worry that this leads to a breakdown of factorization. However, we have seen that factorization is maintained by virtue of certain nontrivial identities. We expect that a similar situation holds for the closed spin chain with four or more holes.

5. Acknowledgements

The work described here was done in collaboration with H. de Vega and M. Grisaru. This work was supported in part by the National Science Foundation under Grant PHY-92 09978.

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Figure Captions

Fig. 1: Ground state of spin 1/2 chain, with $N = 30$. Diamonds denote real roots of the Bethe Ansatz equations.

Fig. 2: $S = S^z = 1$ excited state. Open circles denote holes. (The scale here differs from the one in Fig. 1.)

Fig. 3: $S = S^z = 0$ excited state. The 2-string (denoted by X's) has its center at $(\tilde{\lambda}_1 + \tilde{\lambda}_2)/2$.

Fig. 4: Two-dimensional vertex model. Solid and dashed lines correspond to spin 1/2 and spin 1, respectively. The vertex formed by lines corresponding to spins s_1 and s_2 has weight $R^{(s_1, s_2)}(\lambda)$. (Periodic boundary conditions should be imposed in both horizontal and vertical directions.)

Fig. 5: Ground state of alternating spin 1/2 - spin 1 chain. Diamonds denote real roots (1-strings) and X's denote complex roots (2-strings) of Bethe Ansatz equations.

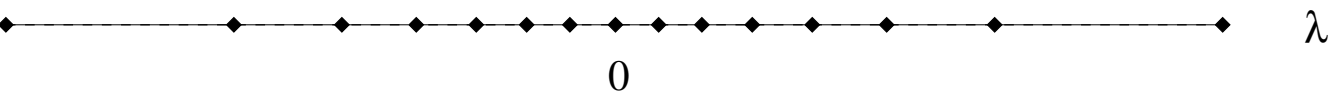
Fig. 6: $S = S^z = 0$ excited state. The center of the 2-string is given by Eq. (4.27).

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